Section 11.3
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NATIONAL BUREAU OF STANDARDS REPORT

5832

Draft of
Part III, Sections 3,4
(Factorial Experiments and
Experiments to Determine
Optimum Conditions)
for

MANUAL ON EXPERIMENTAL STATISTICS
FOR ORDNANCE ENGINEERS

A Report to

OFFICE OF ORDNANCE RESEARCH
DEPARTMENT OF THE ARMY

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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Prepared by
Statistical Engineering Laboratory

A Report to
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NOTICE

This report is a preliminary draft of Part III, sections 3 and 4 for the Manual on Experimental Statistics for Ordnance Engineers. It covers two major topics: factorial experiments and experiments to determine optimum conditions or levels. Taken with sections 1 and 2 (NBS Report 5635) it completes the treatment of Design of Experiments in preliminary draft form.

No known inaccuracies exist in the present draft, but improvements in arrangement and exposition of some of the material may be made at a later time.

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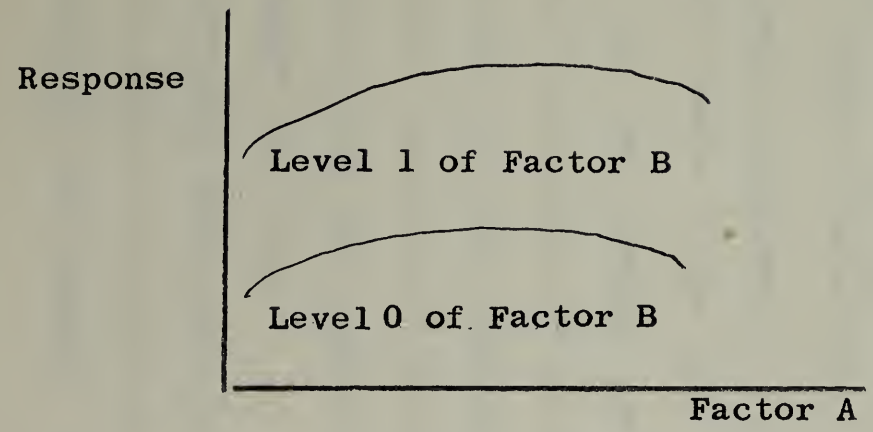
3. Experiments in which Several Factors are Studied Simultaneously (Factorial Experiments)

In many experiments we are interested in the effects of each of several factors. As an example, we may be interested in the effect of pressure and temperature on the yield of a given chemical. The two factors in which we are interested are pressure and temperature. One method of investigating the effect of each of these factors is to first make an investigation of the effect of pressure (for some given temperature), and then to make an investigation of the effect of temperature (for some given pressure). There are several criticisms that may be made of this procedure. In the first place the results may be fragmentary in the sense that we have investigated the effects of differing pressures at one temperature only (also the effects of different temperatures at one pressure only). At another temperature, varying the pressure may affect the yield in a considerably different manner. In statistical language, there may be an "interaction" effect between the two factors in our range of interest, and our procedure does not enable us to detect it. Secondly the procedure is inefficient in that a well planned "factorial" investigation or experiment of the same size as either of the two "one at a time" investigations, could have enabled us to obtain at least as much information about the effect of the two factors.

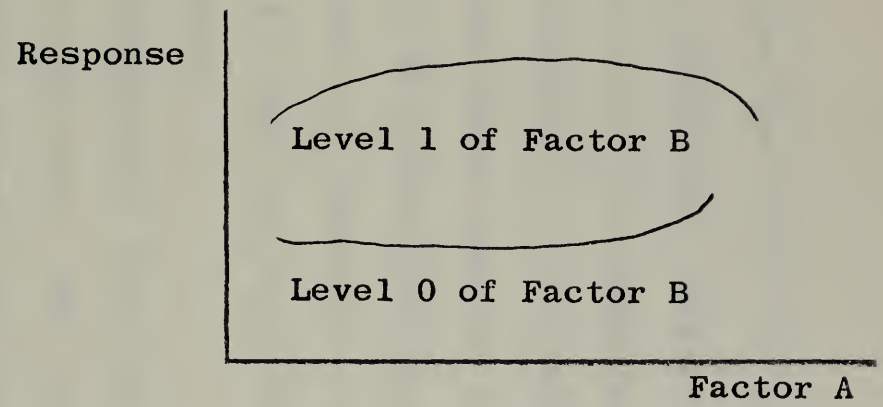
In a factorial experiment, a given number of "levels" of each factor are selected, and a trial is conducted for each combination of levels of all the factors. Suppose in our example, we selected two levels, say 7cm. and 14 cm. for pressure, and two levels, say, 70°F. and 100°F., for temperature. Then there would be four combinations of pressure and temperature, and in our factorial experiments we would have four trials.

In the above discussion, we used the term "levels" in connection with quantitative factors. The term is also used in connection with qualitative factors. In the analysis of factorial experiments, we speak of "Main Effects" and "Interaction Effects" (or simple "Interaction"). If the difference in the response between two levels of factor A is the same regardless of the level of factor B, (except for experimental error) then we say that there is no interaction between A and B, or that the AB interaction is zero. Figure 3 gives examples of response or yield curves, some of which have interaction.

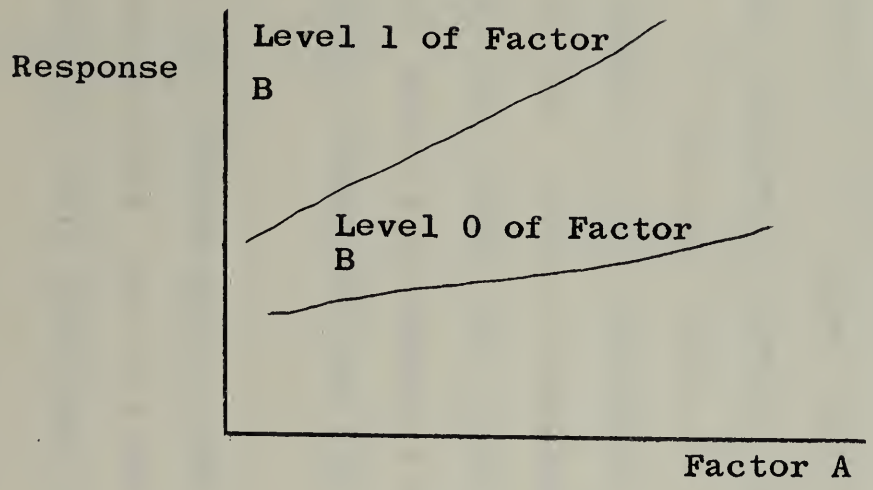
Figure 3



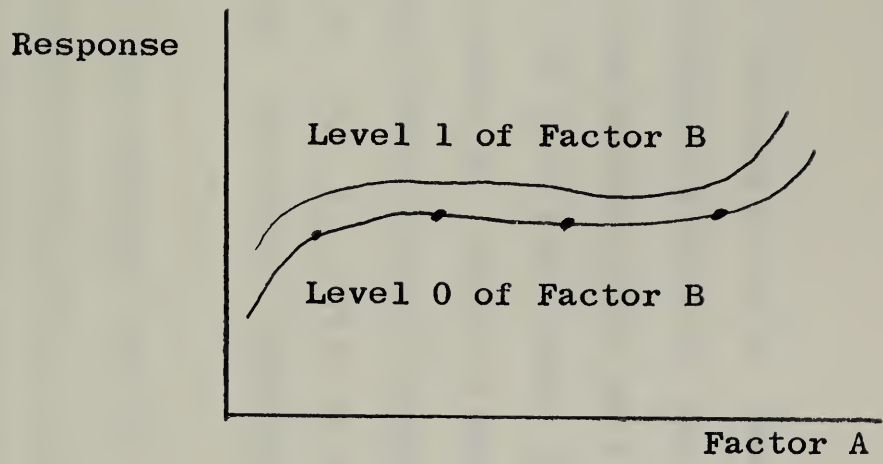
No interaction between Factors A and B



Interaction



Interaction



No Interaction

If we have two levels of each of the factors A and B, then the AB interaction (neglecting experimental error) is the difference in the responses of A at the second level of B minus the difference in the responses of A at the first level of B. If we have more than two levels of either or both of A and B then the AB interaction is composed of more than one component. If we have a levels of the factor A, and b levels of the factor B, then the AB interaction has (a-1)(b-1) independent components.

Interactions involving three or more factors can be defined similarly. For instance, the ABC interaction is the interaction between the factor C and the AB interaction (or equivalently between the factor B and the AC interaction, or A and the BC interaction). Main effects of a given factor are always functions of the average response or yield at the various levels of the main effect. In the case where a factor has two levels, the "Main Effect" is the difference between the average responses at the two levels, averaged over all levels of the other factors. In the case where the factor has more than two levels, then there are several independent components of the main effect, the number being one less than the number of levels.

The case where some or all of the factors are at more than two levels is slightly more complicated, and will not be discussed in this manual. The method is fully described in [2].

3.1 Factorial Experiments Where Each Factor is at Two Levels

A factorial experiment in which we have n factors each at two levels is known as a 2^n factorial experiment. The experiment consists of 2^n trials, one at each combination of levels of the factors. To identify each of the trials, we adopt a conventional notation. A factor is identified by a capital letter, and the two levels of the factor by (1) and the corresponding small letter. If we have three factors A, B and C, then the corresponding levels of the three factors are (1),a; (1),b; and (1),c, respectively. By convention, (1) refers to the lower level, the normal condition, or the absence of a condition. A trial is represented by the product of the levels of the factors in the trial. Thus, the 8 different combinations of levels, or 8 trials are represented by (1), a, b, ab, c, ac, bc, abc. The presence of a small letter means that the factor it represents is at its higher level, and the absence of a letter means that that factor is at its lower level. Thus, (1) denotes the treatment combination with each factor at its lower level, while bc represents the treatment combination with A at its lower level and B and C at their higher level.

For purposes of randomization, the experiment may be regarded as a completely randomized experiment with 2^n treatments. The analysis and interpretation of the results of a 2^n factorial experiment are given in section 3.4.

3.2 Factorial Experiments when Uniform Conditions Cannot be Maintained Throughout the Experiment

When a number of factors are investigated simultaneously, the factorial experiment may be too large to be carried out under uniform conditions, say on one batch of raw material or in one plant in a reasonably short time. In such cases a better procedure is to divide the experiment into 2, 4, 8, etc., groups or blocks, so that the conditions within each of the blocks is as uniform as possible. This procedure will always cause us to confuse information on some effects or interactions, with that of the effect of differences among the blocks. However, it is usually possible to divide the trials so that only three factor and higher-order interactions are confused ("confounded"). Some experimental arrangements for which this is the case are given below. Their analysis and interpretation is given in Section 3.5.1. "Analysis of Blocked Factorial Experiments When Each Factor is at Two Levels".

TABLE 3.2

Experimental Plans When Factorial Experiment Must Be Sub-Divided Into Homogeneous Groups

(The block numbers should be randomized, as well as the treatment combinations within a block.)

Plans for three factors:

i) Four observations per block (ABC confounded).

Block 1	(1),ab,ac,bc
Block 2	a,b,c,abc

Plans for four factors:

i) Eight observations per block (ABCD interaction confounded with block effects).

Block 1	(1),ab,ac,bc,ad,bd,cd,abcd
Block 2	a,b,c,abc,d,abd,acb,bcd

ii) Four observations per block (AD, ABC, BCD confounded with block effects).

Block 1	(1),bc,abd,acd
Block 2	a,abc,bd,cd
Block 3	b,c,ad,abcd
Block 4	d,bcd,ab,ac

Plans for five factors:

i) Sixteen observations per block (ABCDE interaction confounded with block effects).

Block 1	(1),ab,ac,bc,ad,bd,cd,abcd,ae,be, ce,abce,de,abde,acde,bcde
Block 2	a,b,c,abc,d,abd,acd,bcd,e,abe, ace,bce,ade,bde,cde,abcde

TABLE 3.2 (Continued)

Plans for five factors: (Continued)

ii) Eight observations per block (BCE,ADE,ABCD confounded with block effects).

Block 1	(1),ad,bc,abcd,abe,bde,ace,cde
Block 2	a,d,abc,bcd,be,abde,ce,acde
Block 3	b,abd,c,acd,ae,de,abce,bcde
Block 4	e,ade,bce,abcde,ab,bd,ac,cd

iii) Four observations per block (AD,BE,ABC,BCD, DCE,ACE,ABDE confounded with block effects)

Block 1	(1),bce,acd,abde
Block 2	a,abce,cd,bde
Block 3	b,ce,abcd,ade
Block 4	c,be,ad,abcde
Block 5	d,bcde,ac,abe
Block 6	e,bc,acde,abd
Block 7	ab,ace,bcd,de
Block 8	ae,abc,cde,bd

TABLE 3.2 (Continued)

Plans for six factors:

i) Thirty-two observations per block ABCDEF confounded with block effects).

Block 1	all treatment combinations represented by two letters such as ab,ac, etc.
Block 2	(1),abcde, and all treatment combinations represented by three letters such as abc,abd, etc.

ii) Sixteen observations per block (ABCD, BCEF, ADEF confounded with block effects).

Block 1	(1),bc,ad,abcd,ef,bcef,adef,abcdef, bde,cde,abe,ace,bdf,cdf,abf,acf
Block 2	a,abc,d,bcd,aef,abcef,def,bcdef, abde,acde,be,ce,abdf,acdf,bf,cf
Block 3	b,c,abd,acd,bef,cef,abdef,acdef,de, bcde,ae,abce,df,bcdf,af,abcf
Block 4	e,bce,ade,abcde,f,bcf,adf,abcdf,bd, cd,ab,ac,bdef,cdef,abef,acef

iii) Eight observations per block (ADE,BCE,ACF,BDF, ABCD,ABEF,CDEF confounded with block effects).

Block 1	(1),ace,bde,abcd,adf,cdef,abef,bcf
Block 2	a,ce,abde,bcd,df,acdef,bef,abcf
Block 3	b,abce,de,acd,abdf,bcdef,aef,cf
Block 4	c,ae,bcde,abd,acdf,def,abcef,bf
Block 5	d,acde,be,abc,af,cef,abdef,bcdf
Block 6	e,ac,bd,abcde,adef,cdf,abf,bcef
Block 7	f,acef,bdef,abcdf,ad,cde,abe,bc
Block 8	ab,bce,ade,cd,bdf,abcdef,ef,acf

TABLE 3.2 (Continued)

Plans for six factors: (continued)

iv) Four observations per block (AD,BE,CF,ABC,BCD, CDE,DEF,ACE,AEF,ABF,BDF,ABDE,BCEF,ACDF,ABCDEF confounded with block effects).

Block 1	(1),bcef,acdf,abde
Block 2	a,abcef,cdf,bde
Block 3	b,cef,abcdf,ade
Block 4	c,bef,adf,abcde
Block 5	d,bcdef,acf,abe
Block 6	e,bcf,acdef,abd
Block 7	f,bce,acd,abdef
Block 8	ab,acef,bcdf,de
Block 9	ac,abef,df,bcde
Block 10	ad,abcdef,cf,be
Block 11	ae,abcf,cdef,bd
Block 12	af,abce,cd,bdef
Block 13	bc,ef,abdf,acde
Block 14	bf,ce,abcd,adef
Block 15	abc,aef,bdf,cde
Block 16	abf,ace,bcd,def

Plans for seven factors:

i) Sixty-four observations per block (ABCDEFG confounded with block effects).

Block 1	All treatment combinations represented by two letters, four letters or six letters, e.g., ab,abcd,etc.
Block 2	(1) and all treatment combinations represented by three or five letters. plus abcdefg.

TABLE 3.2 (Continued)

Plans for seven factors: (Continued)

ii) Thirty-two observations per block (ABCD,ABEFG, CDEFG confounded with block effects).

Block 1	(1),ab,abcd,ace,acf,acg,ade,adf,adg, bce,bcf,cdef,cdeg,cdfg,abcdef,abcdeg, abcdfg,abef,bcg,bde,bdf,bdg,abeg,abfg, cd,ef,eg,fg,acefg,adefg,bcefg,bdefg
Block 2	a,b,bcd,ce,cf,cg,de,df,dg,abce,abcf, acdef,acdeg,acdfg,bcdef,bcdeg,bcdfg, bef,abcg,abde,abdf,abdg,beg,bfg,acd, aef,aeg,afg,cefg,defg,abcefg,abdefg
Block 3	c,abc,abd,ae,af,ag,acde,acdf,acdg,be, bf,def,deg,dfg,abdef,abdeg,abdfg, abcef,bg,bcde,bcdf,bcdg,abceg,abcfg, d,cef,cfg,aefg,acdefg,befg,bcdefg
Block 4	e,abe,abcde,ac,acef,aceg,ad,adef, adeg,bc,bcef,cdf,cdg,cdefg,abcdf, abcdg,abcdefg,abf,bceg,bd,bdef,bdeg, abg,abefg,cde,f,g,efg,acfg,adfg, bcfg,bdfg

iii) Sixteen observations per block (ABCD,BCEF,ADEF, ACFG,BDFG,ABEG,CDEG, confounded with block effects).

Block 1	(1),bde,adg,abeg,bcg,cdeg,abcd,ace,efg, bdfg,adef,abf,bcef,cdf,abcdefg,acfg
Block 2	a,abde,dg,beg,abcg,acdeg,bcd,ce,aefg, abdfg,def,bf,abcef,acdf,bcdefg,cfg
Block 3	b,de,abdg,aeg,cg,bcdeg,acd,abce,befg, dfg,abdef,af,cef,bcdf,acdefg,abcfg
Block 4	c,bcde,acdg,abceg,bg,deg,abd,ae,cefg, bcdfg,acdef,abcf,bef,df,abdefg,afg
Block 5	d,be,ag,abdeg,bcdg,ceg,abc,acde,defg, bfg,aef,abdf,bcdef,cf,abcefg,acdfg
Block 6	e,bd,adeg,abg,bceg,cdg,abcde,ac,fg, bdefg,adf,abef,bcf,cdef,abcdfg,acefg
Block 7	f,bdef,adfg,abefg,bcfg,cdefg,abcdf,acef, eg,bdg,ade,ab,bce,cd,abcdeg,acg
Block 8	g,bdeg,ad,abe,bc,cde,abcdg,aceg,ef, bdf,adefg,abfg,bcefg,cdfg,abcdef,acf

TABLE 3.2 (continued)

Plans for seven factors: (continued)

iv) Eight observations per block (ACF,ADE,BCE,BDF,CDG, ABG,EFG,ABEF,CDEF,ABCD,BDEG,ACEG,ADFG,BCFG,ABCDEFG confounded with block effects).

Block 1	(1),aceg,bdeg,abcd,adfg,cdef,abef,bcfg
Block 2	a,ceg,abdeg,bcd,dfg,acdef,bef,abcfg
Block 3	b,abceg,deg,acd,abdfg,bcdef,aef,cfg
Block 4	c,aeg,bcdeg,abd,acdfg,def,abcef,bfg
Block 5	d,acdeg,beg,abc,afg,cef,abdef,bcdfg
Block 6	e,acg,bdg,abcde,adefg,cdf,abf,bcefg
Block 7	f,acefg,bdefg,abcdf,adg,cde,abe,bcg
Block 8	g,ace,bde,abcdg,adf,cdefg,abefg,bcf
Block 9	ab,bceg,adeg,cd,bdfg,abcdef,ef,acfg
Block 10	ac,eg,abcdeg,bd,cdfg,adef,bcef,abfg
Block 11	ad,cdeg,abeg,bc,fg,acef,bdef,abcdfg
Block 12	ae,cg,abdg,bcde,defg,acdf,bf,abcefg
Block 13	af,cefg,abdefg,bcdf,dg,acde,be,abcg
Block 14	ag,ce,abde,bcdg,df,acdefg,befg,abcf
Block 15	bg,abce,de,acdg,abdf,bcdefg,aefg,cf
Block 16	abg,bce,ade,cdg,bdf,abcdefg,efg,acf

3.3 Fractional Factorial Experiments

If we have many factors, a complete factorial experiment, where all combinations of levels of factors are investigated involves a large number of tests. This is true even when only two levels of each factor are being investigated. In such cases it is often useful to use a plan which involves

only a fraction of the total number of tests, e.g., a fractional factorial plan. Such plans have the advantage of requiring fewer tests. Further, they do not preclude the possibility of later completing full factorial experiments.

Fractional factorial experiments obviously cannot produce as much information as the completed factorial. However, if the tests included are carefully selected, it is usually possible to sort out the information which is most important. This can be done if we are willing to make the assumptions that a number of effects are zero - for example all interaction effects involving three or more factors. This assumption is often justified, since , experience indicates that it is rare to find an appreciable three-factor interaction effect in a well planned experiment.

In a complete 2^n factorial experiment, there are n main effects, 2^n-n-1 interaction effects and an overall average effect. The 2^n tests can be used to give independent estimates of the 2^n effects. In a fractional factorial experiment (say the fraction $1/2^b$), we have only 2^{n-b} tests, and therefore can make only 2^{n-b} independent estimates. In this case, the plan is designed so that we have 2^{n-b} groups, each consisting of 2^b effects. Further, we can make 2^{n-b} independent estimates, each estimate being a linear combination of the effects included in a group. Effects included in the same group are said to be aliased.

In many instances, it is possible to devise a plan so that each group contains only one main effect or two-factor interaction, and the rest higher-order interactions i.e., main effects and two factor interactions are aliased only with higher order interaction effects. If the assumptions are justified, then our estimates are estimates of main effects or interactions.

If we plan to make tests as to whether or not certain of the effects are significant, then we must have an estimate of the variation due to experimental error which is independent of our estimates of the effects. If we do not have an estimate from previous work or experience, then we must use an estimate from our experiment. To do this, we must decide before conducting the experiment (or at least before having a knowledge of the responses or yields) which of the effects we are estimating may be assumed to be zero, i.e., which of the estimated effects (see plans of Table 3.3) can be used in our estimate of the variation due to experimental error.

Decisions made after examination of the data will generally result in our using the smaller "estimated effects" in our estimate of error, causing α to be greater than its nominal value and resulting in an increased number of conclusions of significant effects and unduly shortened confidence interval estimates. The degrees of freedom in

our estimate s^2 of the variation due to experimental error will be equal to the number of "estimated effects" which we assume are due to experimental error.

Table 3.3 gives a number of useful fractional factorial plans, together with the effects that can be estimated (assuming three-factor and higher order interaction terms are negligible). The treatment combinations should be allocated randomly to the experimental material. Further plans may be found in [5].

TABLE 3.3

Plans	Treatment Combinations	Estimated Effects
Plan 1: Three factors 1/2 replication 4 observations	(1) ac bc ab	T A-BC B-AC -C+AB
Plan 2: Four factors 1/2 replication 8 observations	(1) ad bd ab cd ac bc abcd	T A B AB+CD C AC+BD BC+AD D

TABLE 3.3 (Continued)

Plans	Treatment Combinations	Estimated Effects
Plan 3: Five factors 1/2 replication 16 observations	(1) ae be ab ce ac bc abce de ad bd abde cd acde bcde abcd	T A B AB C AC BC -DE D AD BD -CE CD -BE -AE -E
Plan 4: Five factors 1/4 replication 8 observations	(1) ad bde abe cde ace bc abcd	T A-DE B-CE AB+CD C-BE AC+BD -E+BC+AD D-AE
Plan 5: Six factors 1/4 replication 16 observations	(1) ae bef abf cef acf bc abce df adef bde abd cde acd bcdf abcdef	T A B AB+CE C AC+BE BC+AE+DF E D AD+EF BD+CF * CD+BF * F AF+DE

*) To be used in our estimate of the variation caused by experimental error.

TABLE 3.3 (Continued)

Plans	Treatment Combinations	Estimated Effects
Plan 6: Six factors 1/8 replication 8 observations	(1) adf bde abef cdef ace bcf abcd	T A-DE-CF B-CE-DF AB+CD+EF C-AF-BE -F+AC+BD -E+AD+BC D-AE-BF
Plan 7: Seven factors 1/8 replication 16 observations	(1) aeg befg abf cef acfg bcg abce dfg adef bde abdg cdeg acd bcdf abcdefg	T A B AB+CE+DG C AC+BE+FG BC+AE+DF E D AD+EF+BG BD+CF+AG G CD+BF+EG * F AF+DE+CG
Plan 8: Eight factors 1/16 replication 16 observations	(1) aegh befg abfh cefh acfg bcgh abce dfgh adef bdeh abdg cdeg acdh bcdf abcdefgh	T A B AB+CE+DG+FH C AC+BE+FG+DH BC+AE+DF+GH E D AD+EF+BG+CH BD+AG+CF+EH G CD+AH+BF+EG H F AF+DE+CG+BH

*) To be used in our estimate of the variation caused by experimental error.

3.4 Analysis of Factorial Experiments When Each Factor is at Two Levels

3.4.1. Estimation of Main Effects and Interactions

Yates has outlined a systematic method for obtaining estimates of the main effects and interactions. The method as given here is general, and applies to factorials, blocked factorials and fractional factorials for which we have 2^n observations*. The treatment combinations are given in the first column, and the estimates of the main effects and interactions are given in the last column of Table 3.4.1 (column n+2.) The order in which the treatment combinations are listed in column 1) determines the order in which the estimates are listed in the last column of the table. In the case of fractional factorials, the treatment combinations should be listed in the order given in the plans (see Table 3.3). The last column will then give the estimates of the effects in the order listed in the plans. In the case of factorials or blocked factorials the treatment combinations should be listed in "standard" order, i.e., for two factors the order is (1),a,b,ab; for three factors (1),a,b,ab,c,ac, bc,abc; for four factors (1),a,b,ab,c,ac,bc,abc,d,ad,bd,abd, ...,abcd,etc.

---

*) In fractional factorials we have $2^{n'}$ observations where n'=n-b. See section 3.3.

The estimates of the main effects and interactions then appear in the same order, i.e., T(total),A,B,AB,etc. The systematic procedure is as follows:

i) In the first column of a table with n+2 columns, list the treatment combinations.

ii) In the second column, enter the observed yields or responses corresponding to the treatment combinations of column 1).

iii) In the top half of column 3), enter in order the sums of consecutive pairs of entries in column 2). In the bottom half of the column enter in order the differences between the same consecutive pairs of entries, i.e., second entry minus first entry,,fourth entry minus third entry, etc. (See Table 3.4.1).

iv) Obtain columns 4), 5), ..., n+2) in the same manner as column 3), i.e., by obtaining in each case the sums and differences of the pairs in the preceding column in the manner described in iii).

v) The entries in column n+2) divided by 2^{n-1} are the estimates of the main effects and interactions. We call the entries corresponding to the effects T,A,B,AB,etc., g_T, g_A, g_B, g_{AB} respectively.

TABLE 3.4.1

Estimation of Main Effects and Interactions of a 2^3 factorial by Yates Method

Treatment combinations	Response (Yield)			
(1)	2.9	6.2	15.3	29.6 (Total)
a	3.3	9.1	14.3	2.2 estimate of 4A
b	4.0	5.8	1.5	5.6 " " 4B
ab	5.1	8.5	0.7	-1.0 " " 4AB
c	2.3	0.4	2.9	-1.0 " " 4C
ac	3.5	1.1	2.7	-0.8 " " 4AC
bc	4.5	1.2	0.7	-0.2 " " 4BC
abc	4.0	0.5	-1.7	-2.4 " " 4ABC

Some checks on the computation are as follows:

i) The sum of all the 2^n individual responses should equal the total given in the first entry of the last column.

ii) The sum of the squares of the individual responses should equal the sum of the squares of the entries in the last column divided by 2^n.

iii) For any main effect, the entry in the last column equals the sum of the yields in which that factor is at its higher level minus the sum of the yields in which that factor is at its lower level.

For interval estimates of the main and interaction effects see section 3.4.3.

3.4.2 Testing for Significance of Main Effects and Interaction

Ordinarily, we will not have an independent estimate of the variation introduced as a result of experimental error. It is often possible to assume that the interactions involving 3 factors or more are negligible, and that our estimates of these interactions differ from zero only because of experimental error. (Occasionally we may include two factor interactions when we have reason to believe that they are also negligible).

Our procedure is then as follows:

i) Choose α, the level of significance.

ii) Using the last column, find the sum of the squares of all entries corresponding to interactions of three or more factors*. Divide this sum by $2^n\nu$ where ν is the number of interactions included [$\nu = 2^n - (n^2+n+2)/2$]. This quantity is our estimate s^2 of the variation due to experimental error. (If an independent estimate of the variation due to experimental error is available, say s_1^2, with ν_1 degrees of freedom, then this estimate may be used instead of s^2.)

iii) Look up $q_{1-\alpha}(1,\nu)$ in Table IV.

iv) Compute $w = 2^{(n-1)/2} q_{1-\alpha} s$.

v) For any main effect or interaction X, if $g_X > w$, conclude that X is different from zero, i.e., if $g_A > w$, conclude that the A effect is different from zero. Otherwise, conclude that there is no reason to believe X differs from zero.

---

*) In those cases where it is necessary to use certain two factor interactions for which we have a priori reason to believe the effects are negligible, the sum of squares of these two factor interactions should be included in the sum. The division will then be $2^n\nu$ where ν is the number of interactions used in our estimate of the experimental error.

3.4.3. Interval Estimates of Main Effects and Interactions

If we wish to make a $1-\alpha$ confidence interval estimate of a main effect or interaction effect we may use the calculations of the previous section. The confidence interval for the main effect or interaction X is $(g_X \pm w)/2^{n-1}$.

3.5 Analysis of Blocked Factorial Experiments When Each Factor is at Two Levels

3.5.1. Estimation of Main Effects and Interactions

Yates' procedure as described in 3.4.1 may be used to obtain estimates of the main effects and interactions. The estimates of the interactions which are confounded with blocks may be rather meaningless.

3.5.2. Testing for Significance of Main Effects and Interactions

Ordinarily we will not have an independent estimate of the variation introduced as a result of experimental error. It is then usual to assume that the interactions involving three factors or more are negligible, and that our estimates of these interactions differ from zero only because of experimental error. (Occasionally we may include two factor interactions when we have reason to believe they are also negligible).

The procedure is as follows:

i) Choose α, the level of significance.

ii) Compute the sum of squares of the g_X's corresponding to interactions of three or more factors*. Omit all the interactions which are confounded with blocks. Divide this sum by $2^n\nu$, where ν is the number of interactions included. This quantity is our estimate s^2 of the variation due to experimental error.

iii) Look up $q_{1-\alpha}(1,\nu)$ in Table IV.

iv) Compute $w = 2^{(n-1)/2} q_{1-\alpha} s$.

v) For any main effect or interaction X, if $g_X > w$, conclude that X is different from zero, i.e., if $g_A > w$, conclude that the A effect is different from zero. Otherwise, conclude that there is no reason to believe X differs from zero.

There is of course, little point in making tests on the interactions which are confounded with blocks.

3.5.3. Interval Estimates of Main Effects and Interactions

A $1-\alpha$ confidence interval estimate of the main effect or interaction X is $(g_X \pm w)/2^{n-1}$.

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*) See the footnote of section 3.4.2.

3.6 Analysis of Fractional Factorial Experiments

3.6.1. Estimation of Main Effects and Interactions

The main effects and interactions can be obtained using Yates' systematic procedure which is described in 3.4.1., if we replace n by n', where $n'=n-b$. In column 1 (of the table of $n'+2$ columns which is used in the procedure) the treatment combinations should be listed in the order given in the plan which has been used. The estimates (multiplied by $2^{n'-1}$) of the main effects and interactions will then appear in column $n'+2$ in the order listed in the same plan.

3.6.2. Testing the Significance of the "Estimated" Effects

Ordinarily we will not have an independent estimate of the variation introduced as a result of experimental error. It is then usual to assume that the interactions involving three factors or more are negligible, and that our estimates of these interactions differ from zero only because of experimental error. (Occasionally we may include two-factor interactions when we have reason to believe they are also negligible). The procedure is as follows:

i) Choose α, the level of significance.

ii) Check the lines corresponding to the "estimated effects" which are assumed to be zero. Compute the sums of squares of the corresponding g_i's. Divide this by ν, the number of lines checked, or the number of "estimated effects" which are assumed to be zero. Divide this sum of squares by $2^{n'}$. This quantity is our estimate s^2 of the variation due to experimental error.

iii) Look up $q_{1-\alpha}(1,\nu)$ in Table IV.

iv) Compute $w = 2^{(n'-1)/2} q_{1-\alpha} s$.

v) For any main effect or interaction X, if $g_X > w$, conclude that X is different from zero, i.e., if $g_{A+BC} > w$, conclude that the estimated effect A+BC is different from zero. Otherwise, conclude that there is no reason to believe X differs from zero.

3.6.3. Interval Estimates of "Estimated Effects"

A $1-\alpha$ confidence interval estimate of the "estimated effect" X is given by $(g_X \pm w)/2^{n'-1}$.

4. Experiments to Determine Optimum Conditions or Levels

There are many situations where we wish to maximize (or minimize) some quantity such as yield, profit, etc., which is an unknown function of several independent quantitative variables. In such cases, a method of trial and error, while it may eventually lead to the optimum is frequently slow and wasteful. A systematic procedure has been suggested by Box and Wilson [3] and is being widely applied.

This section gives some recommended designs and a systematic method of analysis. It is thought to be sufficient in scope to be useful in many experimental problems. The general problem of studying response surfaces, however, is more complicated than it appears here. For further study, it is recommended that refs [1], [2] be consulted.

It is assumed that the reader is thoroughly familiar with the preceding section (section 3 on Factorial Experiments). A basic part of a "Box" design is some sort of factorial design (full, blocked, or fractional). The terminology of factorials is used throughout the section and is not redefined here. For example, the reader must specifically understand such terms as blocks, interactions, and effects and must know how to use Yates' method of analysis. The experimentation is begun by conducting trials using values for the

variables which are in the neighborhood of the present operating values of the variables, or failing that in the neighborhood of some values which are hoped to give yields fairly close to the maximum. At this stage, a "first order" design is used. Its purposes are (1) to ascertain whether we are near the maximum yield, and (2) if we are not near the maximum, to indicate how we should change the values of the variables so as to approach the maximum. A first order design enables us to:

i) approximate the yield in the neighborhood of the trials by means of a linear function of the independent variables.

ii) obtain an estimate of the experimental error.

iii) obtain a check on the adequacy of a linear function in approximating the yield in the neighborhood of the trials.

If the analysis of the first order experiment indicates we are not near the maximum, then the proportionate changes we should make in each variable is indicated. In other words, the analysis indicates the direction in which our experimentation should proceed. The distance however, must still be decided by intuition or hunches of the experimenter. A suggestion is that he make trials at several points in the indicated direction, looking for a likely set of variable values about which he should again conduct trials using a first order design.

If after analysis of a first order design indications are that we are near the maximum, then a second order design is superimposed upon the first order design. This enables us to approximate the yields in the neighborhood of our experimental points by an equation of second degree in all of the variables. It is then a matter of arithmetic to differentiate the equation, and to solve for the values of the variables giving us the maximum yield.

The above procedures have been used with success in a number of situations. The method seems best suited when the amount of experimental error is rather small, although its successful use has not been limited to that case.

How to set up the first order design

i) Choose a centre point - a combination of values of variables which shall be a starting point for the design. This is usually chosen to be somewhere in the neighborhood of present operating values of the variables.

ii) Decide upon a design scale unit for each variable. This is a matter for the experimenter's judgment. The intent is that a change of one unit in the scale chosen for any variable should effect the same change in yield. A skillful choice of scale units for the variables may considerably reduce the total amount of experimentation.

iii) The first order designs given are fractional or complete replicates of factorial experiments, with an additional point or points at the centre. The levels of each factor in the factorial are a distance of one scale unit above or below the centre. For designs given in this section, the scale units in the second order design should be the same as those in the first order design upon which it is superimposed.

If one finds it necessary in the investigation to use a first order design a second time (i.e., at another place), experience and knowledge gained from the first time might be used to make a better choice of units.

How to set up the second order design

The second order designs will in every case consist of all the points of the first order design plus an additional part consisting of more centre points and 2k "star" points. The star points are points at which all variables or factors except one are at the same level as the centre or origin. The remaining factor is α scale units above or below the value of that factor at the origin. There will always be 2k star points.

Table 4 lists some suggested designs for k = 2 to k = 7, taken from Box and Hunter [4], where k is the number of independent

variables or factors. The details of the designs are given in the following section.

It will be noted in Table 4 that the first order designs can be arranged in blocks. In some of the designs ($k = 3$ and $k = 4$) the blocking divides the factorial into two half-replicates. In these cases the blocks are called Part I and Part II in the detailed design. When the location of our first order design is considerably removed from the position of the maximum, and when the experimental error is small, Part I of the design is frequently sufficient to supply the information for which the design was intended, i.e., to indicate that we are removed from the maximum, and to indicate the manner in which we should change our variables in order to approach the maximum. In such a situation, it is pointless to use the remaining parts of the design. Instead, the search should proceed as though the full first order design had been completed.

In the other designs, the blocks are simply blocks, and are so labelled in the detailed design. The blocking given is possible but not necessary, and should only be used if it fits the experimental situation.

If the experiment does not lend itself to the blocking arrangement given, the first order design is considered as an ordinary factorial, and of course there is no confounding with blocks.

TABLE 4. SUMMARY OF PLANS

	Number of Independent Variables, k							
	2	3	4	5	5 ($\frac{1}{2}$ rep)	6	6 ($\frac{1}{2}$ rep)	7 ($\frac{1}{2}$ rep)
Plan No.	1	2	3	4a	4b	5a	5b	6
First Order Design								
Number of points from the factorial, n_c	4	8	16	32	16	64	32	64
Number of added centre points, n_{co}	3	4	4	8	6	8	8	8
If blocking is used,								
Number of blocks	1	2	2	4	1	8	2	8
Number of points per block including centre points	7	6	10	10	22	9	20	9
Second Order Design								
Number of centre points	3	2	2	4	1	6	2	4
Number of star points	4	6	8	10	10	12	12	14
α^2	2	2.6667	4	5.6000	4	8	5.6000	8
α	1.4142	1.6330	2	2.3664	2	2.8284	2.3664	2.8284
Total Number of Points in the Design, N	14	20	30	54	33	90	54	90

4.1 Some Plans or Designs for Finding a Maximum or Minimum

We shall use the usual notation of factorial experimentation. In addition, "centre" points will be denoted as 0. It is important that the trials within each block be randomized.

Plan 1 (two independent variables)

$$k = 2$$

$$\mu = .166667 \qquad \lambda = -.083333$$

$$\nu = .010417 \qquad \eta = .125000$$

First order design:

(1), a, b, ab, 0, 0, 0

In analysis of first order design, use Yates' procedure (see section 3.4) with the observations ordered as above, neglecting the centre points. Effects which can be estimated will come out in this order: T, A, B, AB.

Second order design ($\alpha^2 = 2, \quad \alpha = 1.414$)

0, 0, 0, plus the 4 star points

Plan 2 (three independent variables)

$$k = 3$$

$$\mu = .165358 \qquad \lambda = -.057680$$

$$\nu = .005405 \qquad \eta = .070308$$

First order design

Part I (1), ac, bc, ab, 0, 0

Part II c, a, b, abc, 0, 0

The first experiment may consist of Part I only, or of both Parts I and II.

In analysis of first order design, use Yates procedure (see section 3.4) on the observations ordered as above, neglecting the centre points.

If Part I only has been run, the effects which can be estimated come out in this order: T, A-BC, B-AC, AB-C.

If both Parts I and II have been run, the ordering is as follows:

Order of Input Data For the Yates Procedure	Order of Output From Yates Procedure
(1)	T
ac	A
bc	B
ab	AB
c	ABC (Block effect)
a	BC
b	AC
abc	C

Second order design

0, 0 plus the 6 star points ($\alpha^2 = 8/3$, $\alpha = 1.633$)

Plan 3 (four independent variables)

$$k = 4$$

$$\mu = .166667 \qquad \nu = .005208$$

$$\lambda = -.041667 \qquad \eta = .031250$$

First order design:

Part I (1), ad, bd, ab, cd, ac, bc, abcd, 0, 0.

Part II d, a, b, abd, c, acd, bcd, abc, 0, 0.

The first experiment may consist of Part I only, or of both Parts I and II. In analysis of first order design, use Yates' procedure (see section 3.4) on the observations ordered as above, neglecting the centre points.

If Part I only has been run, the effects which can be estimated come out in this order:

T, A, B, AB + CD, C, AC + BD, BC + AD, D.

If both parts I and II have been run, the ordering is as follows:

Order of Input Data For the Yates Procedure	Order of Output From the Yates Procedure
(1)	T
ad	A
bd	B
ab	AB
cd	C
ac	AC
bc	BC
abcd	*
d	ABCD(Blocks)
a	*
b	*
abd	CD
c	*
acd	BD
bcd	AD
abc	D

Second order design

0, 0 plus the 8 star points. ($\alpha^2 = 4$, $\alpha = 2$)

*Interactions composed of three or more factors. Use for estimate of experimental error.

Plan 4a (five independent variables)

$k = 5$

$\mu = .082621$ $\quad \nu = .000818$

$\lambda = -.016026$ $\quad \eta = .015944$

First order design:

Block 1 (1), ad, bc, abcd, abe, bde, ace, cde, 0, 0,

Block 2 a, d, abc, bcd, be, abde, ce, acde, 0, 0

Block 3 b, abd, c, acd, ae, de, abce, bcde, 0, 0

Block 4 e, ade, bce, abcde, ab, bd, ac, cd, 0, 0

In analysis of first order design, use conventional order in the Yates procedure (see section 3.4), ignoring center points. The effects come out in the Yates order, and all effects are estimated except BCE, ADE, ABCD, which are confounded with block effects.

Second order design

0, 0, 0, 0 plus the 10 star points.

$(\alpha^2 = 5.6, \quad \alpha = 2.366)$

Plan 4b (five independent variables, one-half replicate)

$k = 5$

$\mu = .137255 \qquad \nu = .001838$

$\lambda = -.029412 \qquad \eta = .031250$

First order design:

(1), ae, be, ab, ce, ac, bc, abce, de, ad, bd, abde,

cd, acde, bcde, abcd, 0, 0, 0, 0, 0, 0.

In analysis, use the Yates procedure with the observations ordered as above, neglecting the centre points.

Effects which can be estimated come out in this order:

T, A, B, AB, C, AC, BC, -DE, D, AD, BD, -CE, CD,

-BE, -AE, -E

Second order design: ($a^2 = 4$, $a = 2$)

0 plus the 10 star points

Plan 5a (six independent variables)

$$k = 6$$

$$\mu = .066667 \qquad \nu = .000651$$

$$\lambda = -.010417 \qquad \eta = .007813$$

First order design:

Block 1 (1), ace, bde, abcd, adf, cdef, abef, bcf, 0

Block 2 a, ce, abde, bcd, df, acdef, bef, abcf, 0

Block 3 b, abce, de, acd, abdf, bcdef, aef, cf, 0

Block 4 c, ae, bcde, abd, acdf, def, abcef, bf, 0

Block 5 d, acde, be, abc, af, cef, abdef, bcdf, 0

Block 6 e, ac, bd, abcde, adef, cdf, abf, bcef, 0

Block 7 f, acef, bdef, abcdf, ad, cde, abe, bc, 0

Block 8 ab, bce, ade, cd, bdf, abcdef, ef, acf, 0

In analysis of first order design, use conventional order in the Yates procedure (see section 3.4), ignoring center points. The effects come out in the Yates order, and all effects are estimated except ADE, BCE, ACF, BDF, ABCD, ABEF, CDEF, which are confounded with block effects.

Second order design: ($\alpha^2 = 8$, $\alpha = 2.828$)

0, 0, 0, 0, 0, 0 plus the 12 star points.

Plan 5b (six independent variables, one-half replicate)

$k = 6$

$\mu = .099600$ $\nu = .000862$

$\lambda = -.016892$ $\eta = .015944$

First order design:

Block 1 (1), abcd, bcef, adef, abce, de, af, bcdf, ab, cd,

acef, bdef, ce, abde, bf, acdf, 0, 0, 0, 0

Block 2 ac, bd, abef, cdef, be, acde, cf, abdf, bc, ad,

ef, abcdef, ae, bcde, abcf, df, 0, 0, 0, 0

In analysis of first order design order the observations as follows:

(1), af, bf, ab, cf, ac, bc, abcf, df, ad, bd, abdf, cd,

acdf, bcdf, abcd, ef, ae, be, abef, ce, acef, bcef, abce,

de, adef, bdef, abde, cdef, acde, bcde, abcdef.

Apply the Yates procedure on the observations ordered in this way, and the estimated effects will come out in the following order:

T, A, B, AB, C, AC, BC, *, DF, AD, BD, *, CD, *,

*, EF, E, AE, BE, *, CE, *, *, DF, DE, *, *, CF,

ABF = Blocks, BF, AF, F.

*Interactions of 3 or more factors. Use for experimental error.

Second order design: ($\alpha^2 = 5.6$, $\alpha = 2.366$)

0, 0, plus the twelve star points.

Plan 6 (seven independent variables, one-half replicate)

$k = 7$

$\mu = .081818$ $\quad\quad$ $\nu = .000710$

$\lambda = -.011364$ $\quad\quad$ $\eta = .007813$

First order design:

Block 1	(1), adef, bcef, abcd, cdfg, aceg, bdeg, abfg, 0
Block 2	acef, cd, ab, bdef, adeg, fg, abcdfg, bceg, 0
Block 3	adfg, eg, abcdeg, bcfg, ac, cdef, abef, bd, 0
Block 4	cdeg, acfg, bdfg, abeg, ef, ad, bc, abcdef, 0
Block 5	befg, abdg, cg, acdefg, bcde, abcf, df, ae, 0
Block 6	abcg, bcdefg, aefg, dg, abdf, be, acde, cf, 0
Block 7	abde, bf, acdf, ce, abcefg, bcdg, ag, defg, 0
Block 8	bcdf, abce, de, af, bg, abdefg, cefg, acdg, 0

Second order design: ($\alpha^2 = 8$, $\alpha = 2.828$)

0, 0, 0, 0 plus the 14 star points.

In analysis of first order design, order the observations as shown in the first column below. Apply the Yates procedure (see section 3.4.1) and the effects come out in the order listed in the second column below.

Order of Input Data for the Yates Procedure	Order of Output from the Yates Procedure
(1)	T
ag	A
bg	B
ab	AB
cg	C
ac	AC
bc	BC
abcg	ABC (Error)
dg	D
ad	AD
bd	BD
abdg	ABD(Error)
cd	CD
acdg	ACD (Error)
bcdg	BCD (Error)
abcd	EFG (Blocks)
eg	E
ae	AE
be	BE
abeg	ABE (Blocks)
ce	CE
aceg	ACE (Error)
bceg	BCE (Error)
abce	DFG (Error)
de	DE
adeg	ADE (Error)
bdeg	BDE (Error)
abde	CFG (Error)
cdeg	CDE (Blocks)
acde	BFG (Error)
bcde	AFG (Error)
abcdeg	FG
fg	F
af	AF
bf	BF
abfg	ABF (Error)
cf	CF
acfg	ACF (Blocks)
bcfg	BCF (Error)
abcf	DEG (Error)

Order of Input Data for the Yates Procedure	Order of Output from the Yates Procedure
df	DF
adfg	ADF (Error)
bdfg	BDF (Blocks)
abdf	CEG (Error)
cdfg	CDF (Error)
acdf	BEG (Error)
bcdf	AEG (Error)
abcdfg	EG
ef	EF
aefg	AEF (Error)
befg	BEF (Error)
abef	CDG (Error)
cefg	CEF (Error)
acef	BDG (Error)
bcef	ADG (Blocks)
abcefg	DG
defg	DEF (Error)
adef	BCG (Blocks)
bdef	ACG (Error)
abdefg	CG
cdef	ABG (Error)
acdefg	BG
bcdefg	AG
abcdef	G

4.2 Analysis of First and Second Order Designs

4.2.1 Analysis of First Order Designs

The analysis given here assumes that all interactions involving three or more factors are zero. The procedures are valid whether we use Part I, or Parts I and II, of a given plan. We use the following notation:

n_c = number of trials (excluding centre points)

n_{co} = number of centre points

The effects that can be estimated using part or all of any plan are given in section 4.1 along with the plans. To estimate these effects, we may use Yates' procedure which is described in section 3.4.1. The procedure assumes we have 2^n trials, and thus we may determine n from the formula $n_c = 2^n$, where n_c is the number of non-central points in the first order plan.

> NOTE: It is absolutely essential that the observations be put in order as specified where the design is given in 4.1 before applying the Yates procedure. This order is usually different from the standard order described in 3.4.1.

The steps in the analysis are as follows:

i) Order the observations as specified in 4.1 for analysis.

ii) Go through the Yates procedure to obtain values of the g's in column (n + 2). Add an additional column

to write the effects or combinations of effects corresponding to each g, as shown in 4.1 for the particular plan.

iii) Compute b_o, the arithmetic mean of all the observations (including the centre points).

iv) To compute b_A, find the g (g_A) corresponding to the estimated effect A or the estimated effect containing A.

$$b_A = g_A/n_c$$

(If A appears with a negative sign, then b_A has the opposite sign from g_A.)

g_B, g_C, etc. are computed similarly. The best first order or linear expression for the yield y is then:

$$y = b_o + b_A x_A + b_B x_B + \ldots$$

v) To estimate effects of two factor interactions, find the g's corresponding to effects which contain two factor interactions and no main effects, and divide each by n_c.

To ascertain the accuracies of our estimates in iv) and v) it is useful to compute an estimate of experimental error, if it is not already known. For most of the above plans or parts of plans this is possible and is done as follows:

vi) For each block containing n_{co} (≥ 2) centre points, we may get an estimate s^2_{co} of experimental error with $n_{co} - 1$ degrees of freedom, by computing the variance of the values resulting from these centre trials. (Where n_{co} is small, say 2, 3, or 4, a quick method of computing s^2 is to take the differences of all possible different pairs, sum the squares of these differences and divide by $n_{co}(n_{co} - 1)$. For $n_{co} > 4$, the number of possible pairs probably makes this method more cumbersome than the conventional method.)

In most cases, we can get an additional estimate of the experimental error s^2_c by using the g's corresponding to the interactions composed of three or more factors. If there are v such g's, then we can get an estimate with v degrees of freedom by finding the sum of the squares of the g values and dividing it by vn_c. If we have m blocks, the combined estimate s^2 of the experimental error is

$$[(n_{co} - 1)(\text{Sum of the } s^2_{co}) + vs^2_c]/(mn_{co} - m + v).$$

Roughly speaking, if the estimates b_A, b_B, etc., are large compared with experimental error and the two factor interaction effects, indications are that we are not experimenting in the

neighborhood of the maximum and that we should conduct new trials in the direction indicated (see below). Even if the two factor interaction effects are not negligible, if they are small compared with b_A, b_B, etc., we should probably conduct our trials in another region. Otherwise, the first order plan should be completed and analyzed (if it has not already been completed), since indications are that we may be near the maximum. When the first order plan has been completed, run the second order plan and proceed with its analysis.

What to do when the first order plan indicates we are not near the maximum

If a first order plan indicates we are not near the maximum, we should proceed to investigate another region. The direction to move is suggested by the values of b in the equation

$$y = b_o + b_A x_A + b_B x_B + \ldots$$

For example, consider the equation

$$y = 23 + 4 x_A - 2 x_B$$

This equation shows that, if we increase the level of A by 4 scale units, we should decrease the level of B by 2 scale units. The scale units here are the original scale units chosen for A and B respectively, and not the absolute levels of A and B.

Thus starting from our original centre point we should change the levels of the factors as shown by the size and sign of the coefficients

(i. e., if we increase A by 4 scale units, we should decrease B by 2 units). The possible changes can be illustrated in the following table:

	A	B
Original scale unit	1%	2°
b (Estimated change in y per unit change in factor)	4	-2
Unit multiplied by b	4%	-4°
Original centre point	40%	50°

The direction to take in further experimentation is determined as follows: Choose some convenient increment in one of the factors, e. g., 2% in A. Calculate the proportionate changes required in the other variables, e. g., $\frac{2}{4}$ (-4°) in B.

Therefore the path proceeds as follows:

Original centre point		40%	50°
Step	1	42%	48°
	2	44%	46°
	3	46%	44°
	etc.		

Steps 1, 2, 3 etc., are possible steps in the path indicated for approaching the maximum.

Out next experimental trial should be carried out at some step in this path. It need not be conducted at Step 1. If we believe that we are relatively far from the maximum, as evidenced by the numerical yield of y observed in the first order design, then we may wish to skip along to some other step, before conducting a trial. When we have carried out trials at one or more steps along the path, and have found a place that looks like a maximum, we begin a new first order design there. There is now a new origin or centre, and if it is thought desirable, the scale units for one or more factors may be altered.

4. 2. 2 Analysis of Second Order Designs

i) Use Yates procedure on the elements of the first order plan (excluding the centre points) to obtain the g's. If the yields are written in the first column in the order given in the plan, the estimated effects will be in the order stated in the plan. With the exception of g_T, every g corresponds either to a main effect or a two factor interaction. Thus we have g_A, g_{BC}, etc.

ii) Compute a_A, the sum of the yields for the two star points for which all factors are at the origin except A. Compute d_A, the difference of the above two yields, the yield for the trial with the factor A at -a being

subtracted from the yield with the factor A at $+\alpha$.

Compute likewise a_B, d_B; a_C, d_C, etc.

iii) Compute $g'_i = g_i + \alpha d_i$ $\quad i = A, B, \ldots$

iv) Compute $g'_{ii} = g_T + \alpha^2 a_i$, $\quad i = A, B, \ldots$

v) Compute g'_T, the sum of the yields for all the trials in the first and second order experiment.

vi) Compute g_s, the sum of the yields for the noncentral star trials.

vii) Compute $g = kg_T + \alpha^2 g_s$

viii) Compute $b_o = \mu g'_T + \lambda g$

ix) Compute $b_{ii} = \lambda g'_T + \nu g + \eta g'_{ii}$ $\quad i = A, B, \ldots$

x) Compute $b_i = g'_i/(n_c + 2\alpha^2)$

xi) Compute $b_{ij} = g_{ij}/n_c$ $\quad i \neq j = A, B, \ldots$

xii) From the experiment the best quadratic estimate of the yield in terms of the factors or variables is

$$y = b_o + b_A x_A + b_B x_B + \ldots$$
$$+ b_{AA} x_A^2 + b_{BB} x_B^2 + \ldots$$
$$+ b_{AB} x_A x_B + b_{AC} x_A x_C + b_{BC} x_B x_C + \ldots$$

Our estimate of the optimum levels of the factors (provided the equation has a unique maximum) can be found by differentiating the above equation with respect to each of the variates, setting the resulting expressions equal to zero and solving simultaneously for the values of x_A, x_B, ...

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